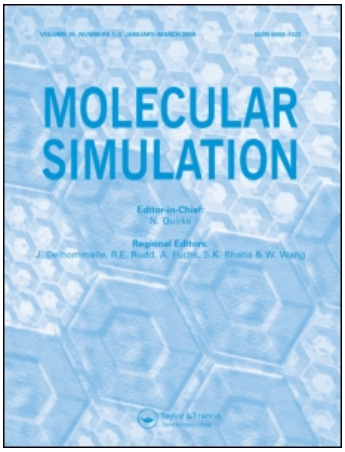

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A compact model to predict quantized sub-band energy levels and inversion layer centroids of MOSFETs with a parabolic potential well approximation

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A compact model to predict quantized sub-band energy levels and inversion layer centroids of MOSFETs with a parabolic potential well approximation

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A compact model to predict sub-band energy levels and inversion charge centroids in the MOSFET surface inversion layer has been presented in this paper for parabolic potential well approximation. Based on a coupled solution of the Schrödinger equation and the Poisson equation following the WKB method, one transcendental equation of the sub-band energy level has been rigorously derived and then the approximate analytical solutions for the sub-band energy levels and the inversion charge centroids have been obtained. The analytical results are compared with the numerical data and a good agreement between the analytical and numerical is found.

1. Introduction

It is well recognized that the traditional silicon MOSFET-based VLSI technology is fast approaching the limit of its performance, and molecular electronics has gained particular attention in recent years because it addresses the ultimate in a nano-scale VLSI system: ultradense and molecular scale [1,2]. Understanding the electron transport mechanism in molecules is very important for the molecular based device applications in the nano-scale VLSI system. Some typical first-principle based methods have been used to study the electron transport in the molecular simulation [3–5]. These methods are, however, computationally expensive for the quantum transport calculation in the molecular simulation. In this case, semi-empirical models and theories are the effective tools to predict the influence of the quantum mechanism effect on the electrical characteristic of the molecular based devices.

In the nano-scale molecular based MOSFETs, the molecular scale implies a high transverse field at the dielectric/molecular semiconductor interface. Such an interface strong field gives rise to the conduction band splitting into discrete sub-bands so as to result in the significant quantization mechanical effects (QMEs). The quantum mechanical effects that the distribution and transport properties of the carriers lead to are quite different from the classic case, e.g. the motion of carriers is not limited in the direction paralleled to the oxide/semiconductor interface but limited in the perpendicular direction, resulting in the different electrical characteristics of MOSFET, e.g. threshold voltage shift, I–V and C–V characteristics.

Rigorous investigation on the carrier transport with the quantized energy levels requires solving the Schrodinger and Poisson equations self-consistently [6,7]. However, the self-consistent solutions are much more complex in procedure realization and expensive in computing time. Thus, the extensive effort was done to develop various approximate methods to include the QMEs. A semi-empirical method is to use an effective bandgap widening to modify the intrinsic carrier density in MOSFET 2-D numerical simulator. However, the difficulty with this method is a lack of exactness and discontinuity [8,9]. A physics-based method is to correct the effective oxide thickness by adding an effective inversion layer centroid. At present, this method becomes more and more popular in *MOSFET modeling* for circuit simulation. In this case, the key is how to accurately obtain the inversion-layer centroid. Traditionally, an approximate inversion layer centroid is obtained by either the variational method and the triangular potential well, or the curve fitting technique

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[10,11]. However, this treatment needs the determination of many parameters and loses the flexibility for different process technologies and MOSFET structures.

In this paper, a novel analytical compact model has been developed to predict the inversion-layer centroid and examine the effects of the different substrate doping and sub-energy levels. Based on a corrected parabolic potential well approximation (CPPWA) and the Wentzel-Kramer-Brillouin (WKB) method [12], a simplified coupled solution of the Poisson and Schrödinger equations are obtained. And then, the approximate analytical expressions of the quantized sub-band energy levels and the inversion layer centroids are derived. The analytical results are compared with the previous numerical analysis and a good agreement is found between both.

2. Physics bases and approximations

The MOSFET with the uniformly doped substrate and (100) oriented p-type silicon is considered here. In fact, the developed model is also available for the other semiconductor materials and the molecular substrate based MOSFETs. Following the semiconductor device physics, the semiconductor energy band bending creates a potential well support by the depletion charge and inversion layer electrons. Since the electrons present in this well occupy a set of energy sub-bands, which distribution energy and wave function should follow the Schrödinger equation

$$\left[-\frac{h^2}{2m^*}\Delta + eV(z)\right]\psi_{ij}(x,y,z) = E_{ij}(x,y)\psi_{ij}(x,y,z) \quad (1)$$

where m^* is the mass tensor, $V(z)$ is the electrostatic potential, and E_{ij} and ψ_{ij} are energy eigenvalue and wave function, respectively, of jth sub-band in ith valley.

The potential $V(z)$ is defined with respect to the potential at the interface and varies with the space charge due to the depletion of hole and, if present, also by the inversion layer electrons. The potential can be calculated from the Poisson equation

$$\frac{\mathrm{d}^2V(z)}{\mathrm{d}z^2} = \frac{e\sum_{ij}\int_{-\infty}^{+\infty}\mathrm{d}z\psi_{ij}(z)\psi_{ij}^*(z)n_{ij} + eN_\mathrm{a}}{\varepsilon_\mathrm{si}} \quad (2)$$

The potential at $z = 0$ or semiconductor surface is defined to be zero and the gradient is taken to be $-E_\mathrm{s}$, the electrical field at the interface. Here N_a represents the background depletion charge density.

Although there are several ways to approach the numerical solution of the Schrödinger equation, we will look at the WKB method of finding the approximate eigenvalues. To solve explicitly the Schrödinger equation, one important classical assumption, the effective mass approximation (EMA), is firstly applied to de-couple 3-D Schrödinger equation into 1-D case that describes the envelope function perpendicular to the interface, $\psi_{ij}(z)$, that constrains the Bloch waves traveling parallel to the interface (x–y plane). And then, the Schrödinger equation (1) is solved approximately by the use of the WKB method. This approach, which is quite accurate, is based on the Bohr theory of quantization of action and is conceptually simple. The Bohr theory postulates that for stable quantum states, the electron motion must have quantized "action", defined as the integral of the momentum over the orbit. In the case of vibration motion bounded on the left conduct edge bottom and right eigenvalue level, or the semiconductor surface inversion layer thickness, which means the inversion layer centroid, the action is defined by the integral of the momentum being those quantized eigenvaue levels from WKB method. In solving the Poisson equation, the CPPWA is used, which assumes that a parabolic potential well is always available either in the depletion or the inversion states and the quantum effect of non-zero inversion layer charge thickness does not change the substrate depletion depth and charge, as shown in figure 1.

In a traditional parabolic potential well case, a surface field is determined by the depletion charges. In the case of CPPWA, the surface field is determined by the combination of depletion charges and inversion layer charges. As a result, the traditional surface field is corrected by adding inversion charge effects so as to result in an effective surface field. Such a treatment greatly simplifies solving the Poisson equation. In the following discussion, an effective surface field expression is followed as the mobility modeling does the common case in order to avoid a complex integral:

$$E_\mathrm{eff} = (Q_\mathrm{B} + \eta Q_\mathrm{inv})/\varepsilon_\mathrm{si} \quad (3)$$

where η is often treated as a constant, being 0.5 for electrons and 0.3 for holes, respectively, in the mobility extraction and characterization. In fact, this parameter has a quantum effect characteristic, which will be discussed later.

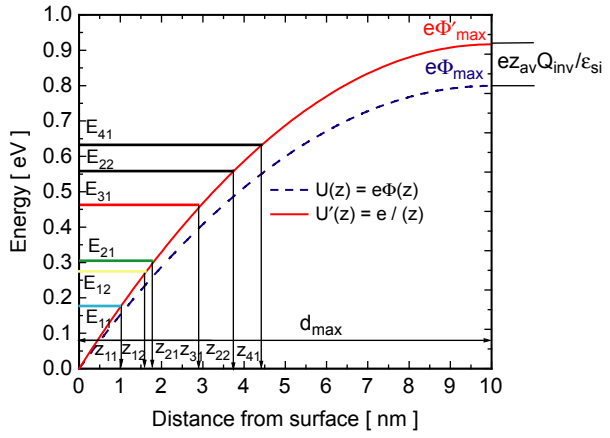

Figure 1. Diagram of the definition of the inversion charge centroid of different energy levels and the effect of the quantum effect on the potential distribution.

An inversion charge centroid is commonly defined as

$$z_{\mathrm{I}} = \int zn\,\mathrm{d}z \Big/ \int n\,\mathrm{d}z \tag{4}$$

This definition features the statistical meaning, it is, however, very difficult to calculate due to that the integral involves an infinite edge. In our treatment, a new physics based inversion charge centroid definition, originally coming from the WKB method, which means the inversion layer centroid is a potential well depth at which an electron eigenvalue is equal to the parabolic potential this depth corresponds to, is used

$$z_I = z_0|_{U'(z_0)=E_{ij}} \tag{5}$$

This new definition is easily determined and is demonstrated the quite same magnitude with the statistics definition to first order approximation. More important, this definition coincides well with the WKB method.

All assumptions above are shown in figure 1, where a classical parabolic well approximation, the CPPWA due to quantum effect and its resulting in sub-band energy levels and the corresponding inversion layer centroids, and the quantum effect contribution to surface potential are all figured.

3. Compact model derivation

Considering a 1-D MOS capacitance case, in a common parabolic potential well case, the electrostatic potential under the *oxide gate* can be written from the depletion approximation

$$\frac{\mathrm{d}^2\phi(z)}{\mathrm{d}z^2} = \frac{eN_{\mathrm{a}}}{\varepsilon_{\mathrm{si}}} \tag{6}$$

Where z is the distance in cm of the semiconductor bulk form the semiconductor surface.

Integrating equation (6) gives

$$\frac{\mathrm{d}\phi(z)}{\mathrm{d}z} = \frac{eN_{\mathrm{a}}}{\varepsilon_{\mathrm{si}}}(z - \mathrm{d}_{\max}) \tag{7}$$

$$\phi(z) = -\frac{eN_{\mathrm{a}}}{2\varepsilon_{\mathrm{si}}}(2z\,\mathrm{d}_{\max} - z^2) = \frac{E_{\mathrm{s}}}{2\mathrm{d}_{\max}}(z^2 - 2z\,\mathrm{d}_{\max}) \tag{8}$$

Where $\mathrm{d}_{\max}$ is the maximum depletion depth in the semiconductor bulk, which is given by

$$\mathrm{d}_{\max} = \frac{Q_{\mathrm{B}}}{N_{\mathrm{a}}} = \sqrt{\frac{4\phi_F\varepsilon_{\mathrm{si}}}{eN_{\mathrm{a}}}} \tag{9}$$

and E_{s} is the surface maximum field, which is expressed as

$$E_{\mathrm{s}} = \frac{eN_{\mathrm{a}}}{\varepsilon_{\mathrm{si}}}\,\mathrm{d}_{\max} = \frac{Q_{\mathrm{B}}}{\varepsilon_{\mathrm{si}}} \tag{10}$$

If we define the carrier energy $U(x) = -e\phi(z)$, the combination equations (7) and (8) gives

$$U(z) = -\frac{eE_{\mathrm{s}}}{2\mathrm{d}_{\max}}(z^2 - 2z\,\mathrm{d}_{\max}) \tag{11}$$

equation (8) results in the magnitude of the maximum electrostatic potential

$$\phi_{\max} = \frac{eN_{\mathrm{a}}\mathrm{d}_{\max}^2}{2\varepsilon_{\mathrm{si}}} \tag{12}$$

where $\phi_{\max}$ is the maximum surface potential without the effect of non-zero thickness of the inversion charges.

Since the inversion charge effect on the surface field is added to that determined by the depletion charges under the CPPWA case, an effective surface field E_{eff} as defined by Sabnis and Clemens, which is the average transverse electrical field in the inversion layer, is used to replace the surface field determined by depletion charges in electrostatic potential and carrier energy expressions for considering the effect of the inversion charges

$$\phi'(z) = -\frac{E_{\mathrm{eff}}}{2\mathrm{d}_{\max}}(2z\,\mathrm{d}_{\max} - z^2) \tag{13}$$

$$U'(z) = -\frac{eE_{\mathrm{eff}}}{2\mathrm{d}_{\max}}(z^2 - 2z\,\mathrm{d}_{\max}) \tag{14}$$

where $\phi'(z)$ and $U'(z)$ are the electrostatic potential and the carrier energy distribution including the effect of non-zero thickness of inversion charges, respectively.

Equations (13) and (14) imply a parabolic potential well in MOSFET surface layer, which is in contrast with the previous triangular potential well approximation, as shown in figure 2. Many numerical analyses reveal that the parabolic potential well is more realistic to the practical case of MOSFETs compared with the triangular potential well approximation.

Comparing the classical depletion approximation under the CPPWA, it is found that the magnitude of the maximum electrostatic potential of the CPPWA slightly increases by $(\eta Q_{\mathrm{in}}\mathrm{d}_{\max}/2)$ due to adding the effect of the inversion charges, which is just the quantum effect, as

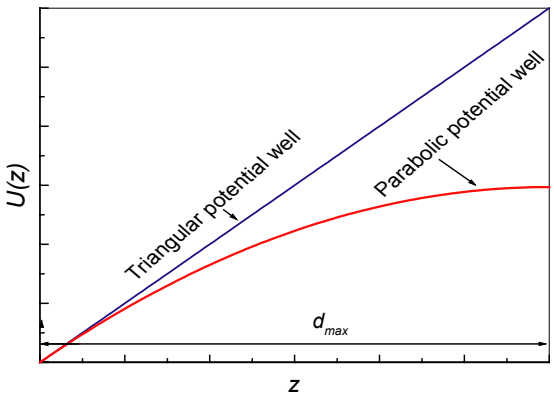

Figure 2. Diagram of the difference between a triangular well potential approximation and a parabolic approximation.

given by equation (13)

$$\phi'_{\max} = \frac{E_{\text{eff}} \mathrm{d}_{\max}}{2} = \frac{eN_a d_{\max}^2}{2\varepsilon_{si}} + \frac{\eta Q_{in} \mathrm{d}_{\max}}{2}$$
$$= \phi_{\max} + \frac{\eta Q_{in} \mathrm{d}_{\max}}{2\varepsilon_{si}} \quad (15)$$

Comparing equation (15) and the influence of the inversion layer centroid on the total band bending on a MOS capacitor as shown in [12] gives

$$\eta = \frac{2z}{\mathrm{d}_{\max}} \quad (16)$$

This expression will be used to determine parameter η.

According to the concept of the WKB method, solving equations (5) and (14) gives the inversion layer centroid:

$$z_I = \mathrm{d}_{\max}\left[1 - \sqrt{1 - \frac{2E_{ij}}{eE_{\text{eff}}\mathrm{d}_{\max}}}\right]$$
$$= \mathrm{d}_{\max}\left[1 - \sqrt{1 - \frac{E_{ij}}{e\phi'_{\max}}}\right] \quad (17)$$

The physical key of the quantum mechanical effects lies in that the energy levels of electrons present in the quantized form. According to the WKB method, the electron wave function is written as

$$\psi_{ij}(z) = \frac{A}{\sqrt{k_{ij}(z)}} \sin\left(\int k_{ij}(z)\,\mathrm{d}z + \frac{\pi}{4}\right) \quad (18)$$

where A is a normalization constant and

$$k_{ij} = \frac{P}{h} = \sqrt{\frac{2m_z(E_{ij} - U'(z))}{h^2}} \quad (19)$$

where h is the Planck constant and P is the electron-quantized momentum.

Since assuming that the inversion electrons are localized in the infinite inversion layer, which should imply that the electron wave function at the semiconductor surface and the maximum inversion layer vanishes, thus the electron wave function is limited only in the parabolic potential well under the WKB approximation. It requires $\sin\left(\int k_{ij}(z)\,\mathrm{d}z + (\pi/4)\right) = 0$ in two classical turning points, thus $\left(\int k_{ij}(z)\,\mathrm{d}z + (\pi/4)\right) = n\pi$ if the integral range is from the semiconductor surface to the maximum inversion layer, namely, from zero to z_I.

After substituting equation (19) into this condition, the following expression is obtained:

$$\int_0^{z_I} \frac{P}{h}\,\mathrm{d}z = n\pi - \frac{\pi}{4} \quad (20)$$

Where n is the quantum level number, $n = 1, 2, 3\ldots6$.

Substitution of equation (17) into (19) to perform the integral of equation (20) gives

$$\mathrm{d}_{\max}\sqrt{\frac{2\mathrm{d}_{\max}E_{ij}}{eE_{\text{eff}}}} + \left(\mathrm{d}_{\max}^2 - \frac{2\mathrm{d}_{\max}E_{ij}}{eE_{\text{eff}}}\right)$$
$$\times\left[\ln\sqrt{\mathrm{d}_{\max}^2 - \frac{2\mathrm{d}_{\max}E_{ij}}{eE_{\text{eff}}}} - \ln\left(\mathrm{d}_{\max} + \sqrt{\frac{2\mathrm{d}_{\max}E_{ij}}{qE_{\text{eff}}}}\right)\right]$$
$$= 2\pi h\left(n - \frac{1}{4}\right)\sqrt{\frac{\mathrm{d}_{\max}}{m_z eE_{ff}}} \quad (21)$$

This expression is a transcendental equation that the inversion electrons in silicon MOS surface layer satisfied. It is evident that E_{ij} is related with the quantum number n, e.g. $E_{ij} = E(n)$. It is very interesting that the inversion thickness can be exactly determined from equation (21) as long as sub-band energy levels are known. However, an analytical solution of equation (21) is impossible to obtain.

Generally, the quantized energy is always less than that in the whole depletion region. In this case, assumption $E_p \le (1/2)eE_{\text{eff}}\mathrm{d}_{\max}$ can give a trial solution of equation (21). The use of this condition simplifies the exponential part of equation (21) via the Taylor expansion:

$$\left[\ln\sqrt{\mathrm{d}_{\max}^2 - \frac{2\mathrm{d}_{\max}E_{ij}}{eE_{\text{eff}}}} - \ln\left(\mathrm{d}_{\max} + \sqrt{\frac{2\mathrm{d}_{\max}E_{ij}}{eE_{\text{eff}}}}\right)\right]$$
$$\approx -\sqrt{\frac{2E_{ij}}{eE_{\text{eff}}\mathrm{d}_{\max}}} \quad (22)$$

Substitution of equation (22) into (21) results in

$$E_{ij} = \left(\frac{e^2E_{\text{eff}}^2h^2}{2m_z}\right)^{\frac{1}{3}}\left[\pi\left(n - \frac{1}{4}\right)\right]^{\frac{2}{3}} \quad (23)$$

Equation (23) is an analytical solution of the sub-band energy levels of 2-D electrons in MOSFET's surface layer with the corrected parabolic potential well.

Combining equations (17) and (23) results in a final expression of the inversion layer centroid

$$z_I = \mathrm{d}_{\max}\left[1 - \sqrt{1 - \frac{[\pi h(2n - 1/2)]^{2/3}}{(em_zE_{\text{eff}})^{1/3}\mathrm{d}_{\max}}}\right]$$
$$= \mathrm{d}_{\max}\left[1 - \sqrt{1 - \frac{E_{ij}}{e\phi'_{\max}}}\right] \quad (24)$$

Moreover, the parameter η is given by solving equations (5) and (24)

$$\eta = 2\left[1 - \sqrt{1 - \frac{[\pi h(2n-1/2)]^{2/3}}{(em_z E_{\text{eff}})^{1/3} \text{d}_{\max}}}\right]$$

$$= 2\left[1 - \sqrt{1 - \frac{E_{ij}}{e\phi'_{\max}}}\right] \quad (25)$$

4. Result and discussion

Figure 2 shows the difference between the triangular well potential and the parabolic potential well approximations. Figure 3 shows the QM sub-band energy level comparisons between the results of the triangular well and the parabolic potential approximations and the numerical result [6,12–13] for the substrate doping 1e17 cm^{-3}. It is evident that the parabolic result is more close to the numerical data.

More interesting is that equation (14) can degrade into the inversion layer centriod expression derived by the variation method [11] if the Taylor expansion is used. The numerical calculation has demonstrated existence of the multiple inversion charge centroids. Figure 4 shows the comparison of the multiple inversion layer centroids of the different sub-band energy level for the substrate doping concentration 1e18 cm^{-3}. It is found, the higher of the sub-band energy level, the larger the inversion layer centroid is. For the device and circuit compact modeling, an average inversion charge centroid is evaluated from this analytical model via the maserjian ruler of the inversion charge centroid, similar to the effective mobility calculation. The result comparison with the numerical solution [10,14] is shown in figure 5. Figure 5 also shows the effect of the different substrate doping concentration on the average inversion centroid, which indicates the higher the substrate doping, the smaller the inversion centroid. More important, this compact model predicts the dependence of the weight factor of the inversion charge in the effective filed expression on the effective field, as shown in figure 6.

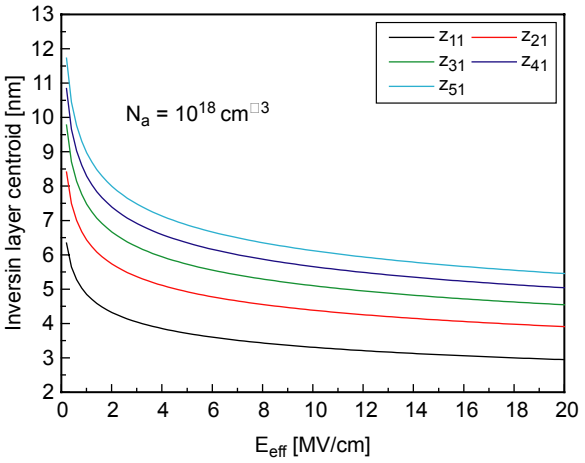

Figure 4. Inversion layer centroids of the different sub-band energy levels versus the effective field.

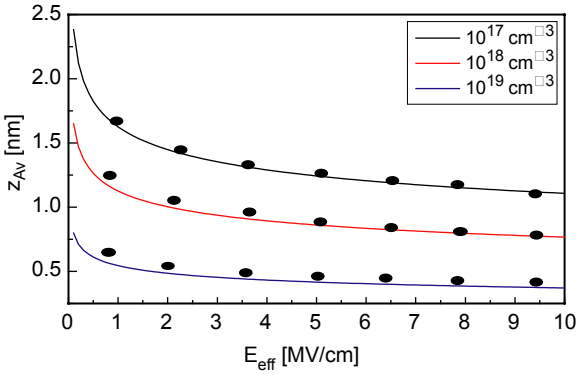

Figure 5. Average inversion layer centroid comparison between the analytic results and the numerical data [5,9].

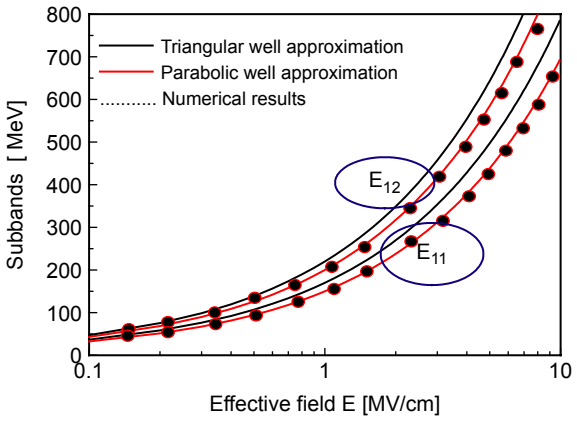

Figure 3. Comparison of the quantized sub-band energy levels predicted by the triangular well potential approximation, the parabolic potential approximation and the self-consistent solution [7,8].

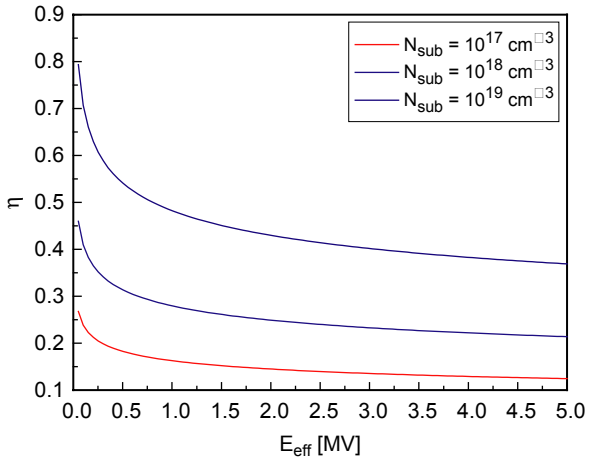

Figure 6. Inversion charge weight factor versus the effective field.

5. Conclusions

A novel analytical model to predict the sub-band energy levels and the inversion charge centroids in MOSFET's surface inversion layer with the parabolic potential well approximation has been presented in this paper. Based on a coupled solution of the Schrödinger equation and the Poisson equation from the WKB method and a parabolic potential well approximation, one transcendental equation of the sub-band energy level has been rigorously derived and then the approximate analytical solutions of the subband energy levels and the inversion charge centroids have been obtained. From our analysis, the effects of the substrate doping concentration and the energy level number on the inversion centroid are predicted and the parameter meaning in the effective field expression is elucidated. Analytic results are compared with the previous numerical analysis and a good agreement is found.

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